Discontinuous Phase Transition in an Exactly Solvable One-Dimensional Creation-Annihilation System

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Abstract

An exactly solvable reaction-diffusion model consisting of first-class particles in the presence of a single second-class particle is introduced on a one-dimensional lattice with periodic boundary condition. The number of first-class particles can be changed due to creation and annihilation reactions. It is shown that the system undergoes a discontinuous phase transition in contrast to the case where the density of the second-class particles is finite and the phase transition is continuous.

One of the most important characteristics of non-equilibrium driven systems is that their steady state consist of current of particles or energy. One-dimensional reaction-diffusion models are examples of such systems which have attracted much attention during last decade [1, 2]. Phase transition and shock formation in these systems are some of their interesting collecting behaviors. These systems have also many applications in different fields of physics and biology. During recent years different models of this type have been studied widely and interesting results have been obtained. The Asymmetric Simple Exclusion Process (ASEP) is a well known example. In this exactly solvable model, which is defined on an open discrete lattice, particle are injected from the left boundary and extracted from the right boundary while hopping on the lattice to the left and to the right randomly. This model has been shown to exhibit non-trivial steady-state phenomena such as phase transitions and shock formation [3]. In order to study the steady state properties of these shocks different models have been proposed. It should be noted that the ASEP is not the only one-dimensional out-of-equilibrium system which exhibits shocks. It has been shown that there are three families of two-states models in which a factorized shock measure is invariant under the time evolution if some constraint on the

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microscopic reaction rates are fulfilled [4]. In [5] the authors have shown that the same phenomenon might also be observed in three-states systems.

In this paper we study an exactly solvable three-states model with non-conserving dynamics on a discrete lattice with a ring geometry. Our model belongs to the class of non-conserving driven-diffusive systems where attachment and detachment of particles are allowed . The study of such models which are variants of the ASEP is motivated by the biological transport processes in living systems [6, 7] and the denaturation transition in DNA [8, 9]. Since our model is based on a newly introduced model in [10], we will first briefly review the main concepts and results of this model. In [10] a non-equilibrium three-species system is introduced on a lattice with periodic boundary condition consisting of the following reaction processes

$$\begin{array}{c} A\emptyset \longrightarrow \emptyset A \quad \text{with rate } \alpha \\ \emptyset B \longrightarrow B\emptyset \quad \text{with rate } \beta \\ AB \longrightarrow BA \quad \text{with rate } 1 \\ A\emptyset \longrightarrow \emptyset\emptyset \quad \text{with rate } \lambda \\ \emptyset\emptyset \longrightarrow A\emptyset \quad \text{with rate } \lambda'. \end{array} \tag{1}$$

As can be seen the number of A particles (first-class particles) is not conserved. In contrast, the number of B particles (second-class particles) is conserved since they only diffuse. It is assumed that in a system with at least one empty site one has finite number of second-class particles with the density ρ_B in the presence of the first-class particles with fluctuating density. It has been shown that in this case a continuous phase transition takes place if the order parameter of the system is taken to be the density of empty sites in the system ρ_E. By taking $\alpha = \beta = 1$ and defining $\omega := \frac{\lambda}{\lambda'}$ it turns out that ρ_E is zero for $\omega < \omega_c$ while it changes linearly as $\rho_E = \frac{\omega}{1+\omega} - \rho_B$ for $\omega > \omega_c$ in which $\omega_c = \frac{\rho_B}{1-\rho_B}$. The current of the second-class is always constant while the particle current of the first-class particles is given by different expressions in each phase. For the case $\alpha \neq 1$ and $\beta = 1$ the transition point is obtained to be $\omega_c = \frac{\rho_B+\alpha-1}{1-\rho_B}$. The density of the empty sites is zero below the transition point while it is given by $\rho_E = \frac{\omega}{1+\omega} - \frac{\omega\rho_B}{1+\omega-\alpha}$ above this point. For $\rho_B \neq 0$ the transition is still continuous.

In present paper we assume that there exists only a single second-class particle in the system which means their density goes to zero in the thermodynamic limit. Second-class or tagged particles are usually introduced to study the dynamical properties of the shocks in one-dimensional driven-diffusive systems; however, one of our major motivations for studying such limiting case is to investigate its effects on the critical behavior of the system and compare it with the previous case in which the density of the second-class particles is non-zero in the thermodynamic limit. As we will see considering this limiting case changes the nature of phase transition from a continuous into a discontinuous one. As far as we know such observation had not been reported before. Apart from the vast applicability of such models in different fields of science (as mentioned above), classification of one-dimensional driven-diffusive models which are exactly solvable using the Matrix Product Formalism (MPF) has been of great interests for

people in this field (for a recent review see [11]). As we will see the model is still exactly solvable using the MPF even in the limiting case $\rho_B \to 0$.
In the following we define $\omega := \frac{\lambda}{\lambda'}$ and apply the MPF [3] to find the partition function of the system. According to the MPF the stationary probability distribution function of any configuration $\mathcal{C}$ of the system of length $L+1$ with a single second-class particle at the site $L+1$ is given by

$$P(\mathcal{C}) = \frac{1}{\mathcal{Z}} Tr[(\prod_{i=1}^{L} \mathbf{X}_i)\mathbf{B}] \tag{2}$$

in which $\mathbf{X}_i = \mathbf{E}$ if the site i is empty otherwise $\mathbf{X}_i = \mathbf{A}$. The normalization factor $\mathcal{Z}$ in the denominator of (2) will be called the partition function of the system. By applying the standard MPF the quadratic algebra of the model is obtained to be [10]

$$\begin{array}{l} \mathbf{AB} = \mathbf{A} + \mathbf{B} \\ \mathbf{AE} = \frac{1}{\alpha}\mathbf{E} \\ \mathbf{EB} = \frac{1}{\beta}\mathbf{E} \\ \mathbf{E}^2 = \frac{\omega}{\alpha}\mathbf{E}. \end{array} \tag{3}$$

By defining $\mathbf{E} = \frac{\omega}{\alpha}|V\rangle\langle W|$ in which $\langle W|V\rangle = 1$ one finds from (3)

$$\begin{array}{l} \mathbf{AB} = \mathbf{A} + \mathbf{B} \\ \mathbf{A}|V\rangle = \frac{1}{\alpha}|V\rangle \\ \langle W|\mathbf{B} = \frac{1}{\beta}\langle W|. \end{array} \tag{4}$$

This quadratic algebra has an infinite-dimensional representation given by the following matrices and vectors

$$\begin{array}{c} \mathbf{A} = \begin{pmatrix} \frac{1}{\alpha} & a & 0 & 0 & \cdots \\ 0 & 1 & 1 & 0 & \\ 0 & 0 & 1 & 1 & \\ 0 & 0 & 0 & 1 & \\ \vdots & & & & \ddots \end{pmatrix}, \mathbf{B} = \begin{pmatrix} \frac{1}{\beta} & 0 & 0 & 0 & \cdots \\ a & 1 & 0 & 0 & \\ 0 & 1 & 1 & 0 & \\ 0 & 0 & 1 & 1 & \\ \vdots & & & & \ddots \end{pmatrix}, \\ |V\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \langle W| = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \end{pmatrix} \end{array} \tag{5}$$

in which $a^2 = \frac{\alpha+\beta-1}{\alpha\beta}$. Since the stationary state of the system without vacancies is trivial, we consider the partition function of the system with at least one empty site which is defined by

$$\mathcal{Z} = Tr[(\mathbf{A}+\mathbf{E})^L\mathbf{B}] - Tr[\mathbf{A}^L\mathbf{B}]. \tag{6}$$

Using (4-6) and after some straightforward calculations we find the following exact expression for the partition function of the system

$$\mathcal{Z} = \frac{\beta+\omega}{\beta(1+\omega-\alpha)}(\frac{1+\omega}{\alpha})^L - \frac{1}{1-\alpha}(\frac{1}{\alpha})^L + \frac{\omega(\alpha+\beta-1)}{\beta(1+\omega-\alpha)(1-\alpha)}. \quad (7)$$

For $\alpha < 1$ there is no phase transition. Assuming $\alpha > 1$ one simply finds the following expressions for the partition function of the system in the large L limit

$$\mathcal{Z} \cong \begin{cases} \frac{\beta+\omega}{\beta(\beta+\omega-\alpha)}(\frac{1+\omega}{\alpha})^L & \text{for } \omega > \alpha - 1 \\ \\ \frac{\omega(\alpha+\beta-1)}{\beta(1+\omega-\alpha)(1-\alpha)} & \text{for } \omega < \alpha - 1. \end{cases} \quad (8)$$

At the transition point the partition function of the system grows like $\mathcal{O}(L)$. Taking the density of the empty sites on the lattice given by

$$\rho_E = \lim_{L\to\infty} \frac{\omega}{L}\frac{\partial}{\partial\omega} \ln \mathcal{Z} \quad (9)$$

as the order parameter of the system, we find using (8) that

$$\rho_E = \begin{cases} \frac{\omega}{1+\omega} & \text{for } \omega > \alpha - 1 \\ \\ 0 & \text{for } \omega < \alpha - 1. \end{cases} \quad (10)$$

At the transition point the density of the empty sites is obtained to be $\rho_E = \frac{\omega}{2(1+\omega)}$. We should note that density of the empty sites for $\omega < \alpha - 1$ drops to zero as $\rho_E \propto \mathcal{O}(\frac{1}{L})$. Discontinuous changes of the density of the empty sites ρ_E in the thermodynamic limit indicates a first-order phase transition in the system. As we mentioned earlier, in the case where the number of the second-class particles on the lattice is finite the density of the empty sites ρ_E changed continuously over the transition point [10].

In order to study the nature of the first-order phase transition one can apply the Yang-Lee theory. Recently it has been shown that the classical Yang-Lee theory can be applied to the out-of-equilibrium systems to study their phase transitions (for a review see [12]). We have calculated the line of the Yang-Lee zeros for our model in the complex-ω plan and found that they lie on a circle of radius α. The center of this circle is at $(-1, 0)$ and intersects the real-ω axis at $Re(\omega) = \alpha - 1$ at an angle $\frac{\pi}{2}$ which again implies a first-order phase transition at the transition point. The density of the zeros has also been found to be a constant all over the circle.

It is also interesting to calculate the density profile of the first class particles on the ring, as seen by the second-class particle, using the MPF. For a system with at least one empty site it is given by

$$\rho_A(i) = \frac{1}{\mathcal{Z}}(Tr[(A+E)^i A(A+E)^{L-i-1}B] - Tr[A^L B]) \quad 0 \le i \le L-1. \quad (11)$$

It turns out that (11) can be calculated exactly using (5) and here are the results in the large L limit

$$\rho_A(i) \cong \begin{cases} \frac{1}{1+\omega} + \frac{\omega(\alpha+\beta-1)}{\alpha(\beta+\omega)} e^{\frac{i-L}{\xi}} & \text{for } \omega > \alpha - 1 \\ \\ 1 - \frac{\alpha-1}{\alpha} e^{-\frac{i}{\xi}} & \text{for } \omega < \alpha - 1 \\ \\ \frac{1}{1+\omega} + \frac{\omega}{1+\omega}(\frac{i}{L}) & \text{for } \omega = \alpha - 1 \end{cases} \tag{12}$$

in which the correlation length is given by $\xi = |\ln(\frac{1+\omega}{\alpha})|^{-1}$. For $\omega > \alpha - 1$ the lattice is filled by first-class particles of density $\frac{1}{1+\omega}$ except just in front of the second-class particle where it increases exponentially to 1. In this phase the density of empty sites is $\frac{\omega}{1+\omega}$. For $\omega < \alpha - 1$ the density of first-class particles increases exponentially from $\frac{1}{\alpha}$ to 1 in the bulk of the lattice. The density of empty sites in this phase is nearly zero in the thermodynamic limit. As can be seen at the transition point the density profile of the particles is linear. This is a sign for a shock however since the number of first-class particles is not a conserved quantity the shock position fluctuates and therefore the resulting profile is linear. This phenomenon has also been observed in the ASEP with open boundaries on the first-order phase transition line where the injection and extraction rates become equal and smaller than one-half. The sock picture will be more clear by calculating the connected two-point function of first-class particles. Straightforward calculations result in the following exact expression which is valid for $i \leq j$ and large system length

$$\begin{aligned} \langle \rho_A(i)\rho_A(j)\rangle_c &:= \langle \rho_A(i)\rho_A(j)\rangle - \langle \rho_A(i)\rangle\langle \rho_A(j)\rangle \\ &\cong -(\tfrac{1}{1+\omega} - \langle \rho_A(i)\rangle)(1 - \langle \rho_A(j)\rangle). \end{aligned} \tag{13}$$

We have also calculated the current of the first-class particles J_A in the steady state. In the large L limit we have found that the current of the first-class particles does not depend on β and is given by

$$J_A = \begin{cases} \frac{\alpha\omega}{(1+\omega)^2} & \text{for } \omega > \alpha - 1 \\ \\ 0 & \text{for } \omega < \alpha - 1 \\ \\ \frac{\omega}{2(1+\omega)} & \text{for } \omega = \alpha - 1. \end{cases} \tag{14}$$

On the other hand, the mean speed of the second-class particle defined as

$$V = \frac{1}{\mathcal{Z}}(\beta Tr[(A+E)^{L-1}EB] + Tr[(A+E)^{L-1}AB] - Tr[A^L B]) \tag{15}$$

can also be calculated exactly. It turns out that V is given by the following exact expression in the thermodynamic limit

$$V = \begin{cases} \frac{\alpha\omega+\beta((1+\omega)^2-\alpha\omega)}{(1+\omega)(\beta+\omega)} & \text{for } \omega > \alpha - 1 \\ \\ 1 & \text{for } \omega \leq \alpha - 1. \end{cases} \tag{16}$$

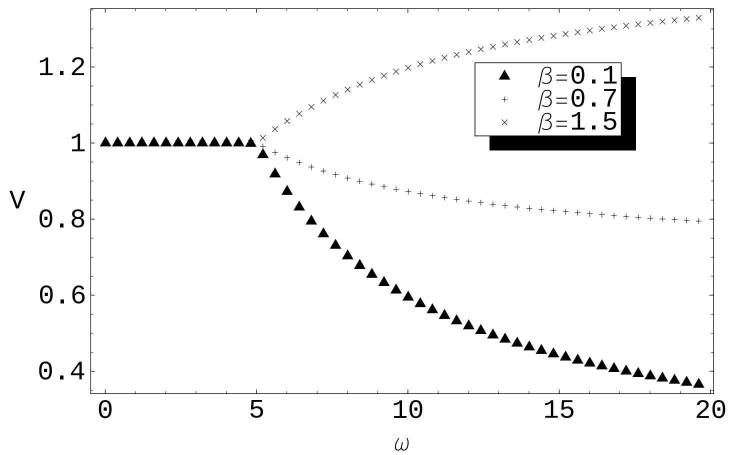

Figure 1: The mean speed of the second-class particle V as a function of ω for three values of β. The length of the system is $L = 100$ and we have chosen $\alpha = 6$.

In Figure 1 we have plotted V as a function of ω for three different values of β on a lattice of length $L = 100$. For $\omega < \alpha - 1$ the speed of the second-class particle is equal to one and does not depend on ω while for $\omega < \alpha - 1$, above the transition point, for $\beta < 1$ ($\beta > 1$) the speed of the second-class particle is a decreasing (increasing) function of ω. For $\beta = 1$ the speed of the second-class particle is always equal to unity.
The model studied in this paper consists of a single second-class particle in the presence of first-class particles with fluctuating density because of creation and annihilation of them. Comparing out results with those obtained in [10] one should note that the order of the phase transition is changed from two to one when the density of the second-class particles goes to zero. The physical explanation for such a macroscopic change can be as follows: for the two cases $\rho_B = 0$ and $\rho_B \neq 0$ and below the critical point there are empty sites on the ring; however, their density goes to zero in the thermodynamic limit. Nevertheless, it is less probable to find configurations of type $A\emptyset$ in the case $\rho_B \neq 0$ (in comparison to the case $\rho_B = 0$) because in this case part of the system is occupied by the second-class particles. Therefore as we increase ω above the critical point it is more probable to create many empty sites in the case $\rho_B = 0$ than the case $\rho_B \neq 0$ because as explained above we have more configurations of type $A\emptyset$ in this case which result in the configuration $\emptyset\emptyset$. This means that as we increase ω above the critical point we expect many empty sites to be created at once in the case $\rho_B = 0$ in contrast to the case $\rho_B \neq 0$ where they are being created slowly.
It is also interesting to compare our results with those obtained in [13] where the

same model as (1) has been considered except it does not contain the creation and annihilation of the first-class particles. It has been shown that the model in this case has two phases: a condensate phase and a fluid phase. Obviously in our model by fixing the number of the first-class particles the phase in which $\rho_E = 0$ will be destroyed; however, a condensate phase emerges in which the density profile of the first-class particles is no longer linear but an step-function and this is in quite agreement with the results in [13].
The MPF enables us to solve some of the one-dimensional driven-diffusive systems exactly; however, by looking at these models we realize that they might have similar quadratic algebras. This means that a quadratic algebra can describe different models with different physical properties and critical behaviors. Now the question is that whether or not other three-states models defined on a ring geometry can be described by (3). In fact we have found that there is a family of such models which are exactly solvable and share the same quadratic algebra [14]. So far two members of this family are introduced and studied in [10] and [15].

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